

A projector-splitting integrator for dynamical low-rank approximation *

Ch. Lubich* and I.V. Oseledets**

*Mathematisches Institut, Universität Tübingen, Auf der
Morgenstelle 10, D-72076 Tübingen, Germany,
lubich@na.uni-tuebingen.de

**Institute of Numerical Mathematics, Russian Academy of
Sciences, Gubkina Street 8, Moscow, Russia,
ivan.oseledets@gmail.com

December 11, 2013

The dynamical low-rank approximation of time-dependent matrices is a low-rank factorization updating technique. It leads to differential equations for factors of the matrices, which need to be solved numerically. We propose and analyze a fully explicit, computationally inexpensive integrator that is based on splitting the orthogonal projector onto the tangent space of the low-rank manifold. As is shown by theory and illustrated by numerical experiments, the integrator enjoys robustness properties that are not shared by any standard numerical integrator. This robustness can be exploited to change the rank adaptively. Another application is in optimization algorithms for low-rank matrices where truncation back to the given low rank can be done efficiently by applying a step of the integrator proposed here.

1 Introduction

Low-rank approximation of large matrices and tensors is a basic model reduction technique in a wide variety of applications ranging from quantum physics to information retrieval. In the present paper, we consider the low-rank approximation of time-dependent matrices $A(t)$, $t_0 \leq t \leq \bar{t}$, which are either given explicitly or are the unknown solution of a differential equation $\dot{A}(t) = F(A(t))$. In the first case, instead of performing an (expensive) low-rank approximation via singular value

*This work was partially supported by DFG, SPP 1324, by RFBR grants 12-01-00546-a, 11-01-00549-a, 12-01-33013 mol-ved-a, RFBR-DFG grant 12-01-91333, by Federal program “Scientific and scientific-pedagogical personnel of innovative Russia”(contracts 14.740.11.1067, 16.740.12.0727, grants 8500 and 8235)

decompositions independently for every t , one would prefer a computationally inexpensive updating procedure that works only with the increments of A and is free from decompositions of large matrices. In the second case, one would like to find an approximate solution to the differential equation working only with its low-rank approximation.

Both cases can be dealt with by *dynamical low-rank approximation* where $A(t)$ is approximated by $Y(t)$ of fixed rank r by imposing that its time derivative should satisfy

$$\|\dot{Y}(t) - \dot{A}(t)\| = \min, \quad (1)$$

where the minimization is over all matrices that are tangent to $Y(t)$ on the manifold \mathcal{M}_r of matrices of rank r , and the norm is the Frobenius norm. In the case of a differential equation $\dot{A} = F(A)$, the above minimization is replaced with

$$\|\dot{Y}(t) - F(Y(t))\| = \min. \quad (2)$$

In both cases, this leads to a differential equation on the manifold of matrices of a given rank r , which is then solved numerically.

For large time-dependent matrices, this approach was proposed and analyzed in [5], and first numerical applications were given in [12]. The approach and its error analysis were extended to tensors in the Tucker format in [6]. Very recently, in [1, 8, 14] the dynamical low-rank approximation approach was extended to tensors in the tensor train (TT) format studied in [13] and the hierarchical Tucker (HT) format studied in [3]. In quantum dynamics, such an approach was used previously in the multiconfiguration time-dependent Hartree (MCTDH) method [10, 11] to determine an approximate solution to the time-dependent multi-particle Schrödinger equation, and the above minimization process is known there as the Dirac–Frenkel time-dependent variational principle (see, e.g., [7]).

The dynamical low-rank approximation leads to differential equations that need to be solved numerically. In this paper we present a numerical integration technique that is fully explicit and, in contrast to standard integrators such as (explicit or implicit) Runge–Kutta methods, does not suffer from a possible ill-conditioning of certain matrices arising in the differential equations. This new method is based on a splitting of the projector onto the tangent space of the low-rank manifold at the current position. A different splitting algorithm was recently proposed in [14], where the differential equations are split along different components. The projector splitting discussed here offers, however, several advantages: it leads to a much simpler and less expensive time-stepping algorithm and it can be shown to enjoy remarkable robustness properties under the ill-conditioning mentioned before.

In Section 2 we recapitulate the dynamical low-rank approximation of matrices, and in Section 3 we describe the novel splitting integrator. In Section 4 we analyze the robustness under over-approximation, that is, under the dreaded ill-conditioning mentioned above. Section 5 presents numerical experiments. The final section addresses some perspectives for the use of the proposed integrator and extensions.

2 Dynamical low-rank approximation of matrices

Let r be a given rank, and let \mathcal{M}_r denote the manifold of all real $m \times n$ matrices of rank r (typically, $r \ll m, n$). In the dynamical low-rank approximation to matrices $A(t) \in \mathbb{R}^{m \times n}$, the approximation

$Y(t) \in \mathcal{M}_r$ is represented in a non-unique way as

$$Y(t) = U(t)S(t)V(t)^\top, \quad (3)$$

where $U(t) \in \mathbb{R}^{m \times r}$ and $V(t) \in \mathbb{R}^{n \times r}$ each have r orthonormal columns, and $S(t) \in \mathbb{R}^{r \times r}$ is an invertible matrix. This looks similar to the singular value decomposition, but $S(t)$ is not assumed diagonal.

It is shown in [5, Prop. 2.1] that, given such a decomposition $Y_0 = U_0 S_0 V_0^\top$ of the starting value and imposing the gauge conditions

$$U(t)^\top \dot{U}(t) = 0, \quad V(t)^\top \dot{V}(t) = 0, \quad (4)$$

the solution $Y(t) \in \mathcal{M}_r$ to the time-dependent variational principle (1) admits a unique decomposition (3), and the factors $U(t), S(t), V(t)$ satisfy the following system of differential equations:

$$\begin{aligned} \dot{U}(t) &= (I - U(t)U(t)^\top) \dot{A}(t) V(t) S(t)^{-1} \\ \dot{V}(t) &= (I - V(t)V(t)^\top) \dot{A}(t)^\top U(t) S(t)^{-\top} \\ \dot{S}(t) &= U(t)^\top \dot{A}(t) V(t). \end{aligned} \quad (5)$$

This system of differential equations is to be solved numerically. The numerical solution of (5) by standard integrators (e.g., of Runge–Kutta type) becomes cumbersome if $S(t)$ is nearly singular. This situation occurs in the case of *over-approximation*, when the true rank of the solution (or approximate rank) is smaller than the chosen rank r . This is a realistic case: the effective rank may not be known in advance, and it is often reasonable to overestimate the rank for accurate approximation. To avoid the possible singularity of $S(t)$ usually some sort of regularization is used. However, such a regularization introduces errors that are poorly understood.

The minimization condition (1) states that at an approximation $Y(t) \in \mathcal{M}_r$, the derivative $\dot{Y}(t)$ is obtained by orthogonally projecting $\dot{A}(t)$ onto the tangent space $T_{Y(t)} \mathcal{M}_r$ of the rank- r manifold at $Y(t)$:

$$\dot{Y}(t) = P(Y(t)) \dot{A}(t), \quad (6)$$

where $P(Y)$ is the orthogonal projector onto the tangent space $T_Y \mathcal{M}_r$ of the manifold \mathcal{M}_r at $Y \in \mathcal{M}_r$. The projector has a simple representation [5, Lemma 4.1]: for $Y = USV^\top$ as in (3),

$$P(Y)Z = ZVV^\top - UU^\top ZVV^\top + UU^\top Z. \quad (7)$$

Note that UU^\top is the orthogonal projector onto the range $\mathcal{R}(Y)$ of $Y = USV^\top$, and VV^\top is the orthogonal projector onto the range $\mathcal{R}(Y^\top)$, so that we can also write

$$P(Y)Z = ZP_{\mathcal{R}(Y^\top)} - P_{\mathcal{R}(Y)} Z P_{\mathcal{R}(Y^\top)} + P_{\mathcal{R}(Y)} Z. \quad (8)$$

3 The integrator

3.1 First-order splitting method, abstract formulation

Let a rank- r approximation Y_0 to $A(t_0)$ be given and consider a step of the standard Lie–Trotter splitting of (6) with (8) from t_0 to $t_1 = t_0 + h$:

1. Solve the differential equation $\dot{Y}_I = \dot{A}P_{\mathcal{R}(Y_I^\top)}$ with initial value $Y_I(t_0) = Y_0$ on the interval $t_0 \leq t \leq t_1$.
2. Solve the differential equation $\dot{Y}_{II} = -P_{\mathcal{R}(Y_{II})}\dot{A}P_{\mathcal{R}(Y_{II}^\top)}$ with initial value $Y_{II}(t_0) = Y_I(t_1)$ on the interval $t_0 \leq t \leq t_1$.
3. Solve the differential equation $\dot{Y}_{III} = P_{\mathcal{R}(Y_{III})}\dot{A}$ with initial value $Y_{III}(t_0) = Y_{II}(t_1)$ on the interval $t_0 \leq t \leq t_1$.

Finally, take $Y_1 = Y_{III}(t_1)$ as an approximation to $Y(t_1)$, the solution of (6) at t_1 . By standard theory, this is a method of first-order accuracy. Remarkably, each of the split differential equations can be solved exactly in a trivial way.

Lemma 3.1. *The solution of 1. is given by*

$$Y_I(t) = U_I(t)S_I(t)V_I(t) \quad \text{with} \quad (U_I S_I)^\bullet = \dot{A}V_I, \quad \dot{V}_I = 0. \quad (9)$$

The solution of 2. is given by

$$Y_{II}(t) = U_{II}(t)S_{II}(t)V_{II}(t) \quad \text{with} \quad \dot{S}_{II} = -U_{II}^\top \dot{A}V_{II}, \quad \dot{U}_{II} = 0, \quad \dot{V}_{II} = 0. \quad (10)$$

The solution of 3. is given by

$$Y_{III}(t) = U_{III}(t)S_{III}(t)V_{III}(t) \quad \text{with} \quad (V_{III}S_{III}^\top)^\bullet = \dot{A}^\top U_{III}, \quad \dot{U}_{III} = 0. \quad (11)$$

Proof. We first notice that each of the terms on the right-hand side of (8) is in the tangent space $T_Y \mathcal{M}_r$, because for the first term the orthonormality $V^\top V = I$ yields

$$P(Y)(ZVV^\top) = ZVV^\top + UU^\top ZVV^\top - UU^\top ZVV^\top = ZVV^\top,$$

so that $ZVV^\top \in T_Y \mathcal{M}_r$. Similarly we also have $UU^\top Z \in T_Y \mathcal{M}_r$ and $UU^\top ZVV^\top \in T_Y \mathcal{M}_r$. It therefore follows that the solutions of 1.-3. all stay of rank r . Hence, $Y_I(t)$ can be factorized as $Y_I(t) = U_I(t)S_I(t)V_I(t)$ with an invertible $s \times s$ matrix S_I and U_I, V_I having orthonormal columns. All the matrices can be chosen to be differentiable, and we thus have

$$\dot{Y}_I = (U_I S_I)^\bullet V_I^\top + (U_I S_I) \dot{V}_I^\top$$

which by 1. must equal $\dot{Y}_I = \dot{A}V_I V_I^\top$. We observe that this is satisfied if $(U_I S_I)^\bullet = \dot{A}V_I$ and $\dot{V}_I = 0$.

The proofs for Steps 2. and 3. are similar. \square

3.2 First-order splitting method, practical algorithm

Lemma 3.1 leads us to the following algorithm. Given a factorization (3) of the rank- r matrix $Y_0 = U_0 S_0 V_0^\top$ and denoting the increment $\Delta A = A(t_1) - A(t_0)$, one step of the integrator reads as follows:

1. Set

$$K_1 = U_0 S_0 + \Delta A V_0$$

and compute the factorization

$$U_1 \hat{S}_1 = K_1$$

with U_1 having orthonormal columns and an $r \times r$ matrix \hat{S}_1 (using QR or SVD).

2. Set

$$\widetilde{S}_0 = \widehat{S}_1 - U_1^\top \Delta A V_0.$$

3. Set

$$L_1 = V_0 \widetilde{S}_0^\top + \Delta A^\top U_1$$

and compute the factorization

$$V_1 S_1^\top = L_1,$$

with V_1 having orthonormal columns and an $r \times r$ matrix S_1 (using QR or SVD).

The algorithm computes a factorization of the rank- r matrix

$$Y_1 = U_1 S_1 V_1^\top,$$

which is taken as an approximation to $Y(t_1)$. Note that Y_1 is identical to the result of the abstract splitting algorithm of Section 3.1, without any further approximation.

3.3 Higher-order schemes

Higher-order extensions can be obtained from the above first-order algorithm by the standard technique of composition rules. The usual symmetric composition is obtained by first taking a step of the above integrator with step size $h/2$ followed by taking its steps in reverse order. The resulting scheme looks as follows (here $A_0 = A(t_0)$, $A_{1/2} = A(t_0 + \frac{h}{2})$, $A_1 = A(t_0 + h)$):

$$\begin{aligned} K_{1/2} &= U_0 S_0 + (A_{1/2} - A_0) V_0, \\ (U_{1/2}, \widehat{S}_{1/2}) &= \text{QR}(K_{1/2}), \\ \widetilde{S}_0 &= \widehat{S}_{1/2} - U_{1/2}^\top (A_{1/2} - A_0) V_0, \\ L_1 &= V_0 \widetilde{S}_0^\top + (A_1 - A_0)^\top U_{1/2}, \\ (V_1, \widehat{S}_1^\top) &= \text{QR}(L_1), \\ \widetilde{S}_{1/2} &= \widehat{S}_1 - U_{1/2}^\top (A_1 - A_{1/2}) V_1, \\ K_1 &= U_{1/2} \widetilde{S}_{1/2} + (A_1 - A_{1/2}) V_1, \\ (U_1, S_1) &= \text{QR}(K_1), \\ Y_1 &= U_1 S_1 V_1^\top. \end{aligned} \tag{12}$$

This symmetrized splitting is a second-order scheme for (6). Higher-order schemes are obtained by suitable further compositions; see, e.g., [4, 9].

3.4 The integrator for matrix differential equations

The basic first-order scheme extends straightforwardly to an explicit method for the low-rank approximation of solutions $A(t)$ of matrix differential equations $\dot{A} = F(A)$, where now $A(t)$ is not known beforehand. The only change is that $\Delta A = A(t_1) - A(t_0)$ is replaced, in a way resembling the explicit Euler method, with

$$\Delta A = hF(Y_0).$$

The symmetric composition with the adjoint method now yields an implicit method. An explicit method of order 2 is obtained by first taking a step with the basic first-order integrator, which

yields an approximation \tilde{Y}_1 , and then to take a step with the above second-order method in which $\dot{A}(t)$ is replaced, at $t = t_0 + \theta h$, with the linear function $B(t_0 + \theta h) = (1 - \theta)F(Y_0) + \theta F(\tilde{Y}_1)$, and correspondingly $A(t)$ with the quadratic function $Y_0 + \int_{t_0}^t B(s) ds$, that is,

$$A(t_0 + \theta h) \approx Y_0 + h \int_0^\theta B(t_0 + \vartheta h) d\vartheta = Y_0 + \frac{h}{2} \theta (2 - \theta) F(Y_0) + \frac{h}{2} \theta^2 F(\tilde{Y}_1).$$

Higher-order methods can again be obtained by composition of steps of the second-order method.

4 Robustness under over-approximation

The equations of motion (5) break down when S becomes singular, and standard numerical integrators applied to (5) run into problems with stability and accuracy when S is ill-conditioned. Such a situation arises when the matrix $A(t)$ to be approximated by a rank- r matrix has rank less than r , or is close to a rank-deficient matrix. It is a remarkable property of the integrator proposed here that it behaves much better than a standard integrator applied to (5) in such a situation of over-approximation. On the one hand, this is already apparent from the observation that there is no matrix inversion in the algorithm. There is in fact more to it.

The following result depends on the ordering of the splitting of the projector (8), so that we first compute $K = US$, then S , then $L = VS^\top$. For a different ordering, such as computing subsequently K, L, S , the following surprising exactness result is not valid.

Theorem 4.1. *Suppose that $A(t)$ has rank at most r for all t . With the initial value $Y_0 = A(t_0)$, the splitting algorithm of Section 3.2 is then exact: $Y_1 = A(t_1)$.*

Proof. We decompose $A(t) = U(t)S(t)V(t)^\top$, where both $U(t)$ and $V(t)$ have r orthonormal columns, and $S(t)$ is an $r \times r$ matrix. We assume that $V(t_1)^\top V(t_0)$ is invertible. If this is not satisfied, then we make the following argument with a small perturbation of $A(t_1)$ such that $V(t_1)^\top V(t_0)$ becomes invertible, and let the perturbation tend to zero in the end.

The first substep of the algorithm, starting from $Y_0 = U_0 S_0 V_0^\top = U(t_0)S(t_0)V(t_0)^\top = A(t_0)$, yields

$$U_1 \hat{S}_1 = A(t_1) V_0 = U(t_1) S(t_1) (V(t_1)^\top V(t_0)),$$

so that the range of

$$A_1 = A(t_1) = (U(t_1) S(t_1)) V(t_1)^\top = U_1 \hat{S}_1 (V(t_1)^\top V(t_0))^{-1} V(t_1)^\top$$

is contained in the range of U_1 , and hence we have

$$U_1 U_1^\top A_1 = A_1, \quad \text{as well as } A_0 V_0 V_0^\top = A_0.$$

Using the formulas of the splitting scheme we then calculate

$$\begin{aligned} Y_1 &= U_1 S_1 V_1^\top \\ &= U_1 \tilde{S}_0 V_0^\top + U_1 U_1^\top \Delta A \\ &= U_1 \hat{S}_1 V_0^\top - U_1 U_1^\top \Delta A V_0 V_0^\top + U_1 U_1^\top \Delta A \\ &= U_0 S_0 V_0^\top + \Delta A V_0 V_0^\top - U_1 U_1^\top \Delta A V_0 V_0^\top + U_1 U_1^\top \Delta A \\ &= A_0 + A_1 V_0 V_0^\top - A_0 - A_1 V_0 V_0^\top + U_1 U_1^\top A_0 + A_1 - U_1 U_1^\top A_0 = A_1, \end{aligned}$$

which is the stated result. □

Consider now a small perturbation to a matrix of rank less than r : with a small parameter ε , assume that (with primes as notational symbols, not derivatives),

$$A(t) = A'(t) + \varepsilon A''(t) \quad \text{with } \text{rank}(A'(t)) = q < r,$$

where A' and A'' and their derivatives are bounded independently of ε . We factorize

$$A'(t) = U'(t)S'(t)V'(t)^\top$$

with $U'(t)$ and $V'(t)$ having q orthonormal columns and with an invertible $q \times q$ matrix $S'(t)$.

We apply the splitting integrator for the dynamical rank- r approximation of $A(t)$ with starting value

$$Y_0 = A'(t_0) + \varepsilon A''_0, \quad \text{rank}(Y_0) = r,$$

where A''_0 is bounded independently of ε (but may differ from $A''(t_0)$). We compare the result of the rank- r algorithm with that of the rank- q algorithm starting from

$$\bar{Y}_0 = A'(t_0) + \varepsilon \bar{A}''_0, \quad \text{rank}(\bar{Y}_0) = q < r.$$

Theorem 4.2. *In the above situation, let Y_n and \bar{Y}_n denote the results of n steps of the splitting integrator for the rank- r approximation and rank- q approximation, respectively, applied with step size h . Then, as long as $t_0 + nh \leq T$,*

$$\|Y_n - \bar{Y}_n\| \leq C(\varepsilon + h),$$

where C is independent of n , h and ε (but depends on $T - t_0$).

We note that by the standard error estimates of splitting methods, the integration error of the rank- q approximation is $\bar{Y}_n - \bar{Y}(t_n) = O(h^p)$, uniformly in ε , for the integrator of order p . Furthermore, it follows from the over-approximation lemma in [5], Section 5.3, that the difference of the rank- r and rank- q approximations is bounded by $Y(t) - \bar{Y}(t) = O(\varepsilon)$.

Proof. (a) We factorize

$$Y_0 = U_0 S_0 V_0^\top,$$

where $U_0 = (U'_0, U''_0) \in \mathbb{R}^{m \times r} = \mathbb{R}^{m \times q} \times \mathbb{R}^{m \times (r-q)}$ and $V_0 = (V'_0, V''_0) \in \mathbb{R}^{n \times r} = \mathbb{R}^{n \times q} \times \mathbb{R}^{n \times (r-q)}$ have orthonormal columns. S_0 is chosen as an $r \times r$ matrix in block-diagonal form

$$S_0 = \begin{pmatrix} S'_0 & 0 \\ 0 & S''_0 \end{pmatrix} \quad \text{with } S'_0 = S'(t_0) \text{ and } S''_0 = O(\varepsilon).$$

We consider the differential equation in the first splitting step, $\dot{Y}_I(t) = \dot{A}(t)P_{\mathcal{R}(Y_I^\top(t))}$. We factorize (omitting the subscript I and the argument t)

$$Y = USV^\top,$$

where U and V have r orthonormal columns, so that we have the equation

$$\dot{U}SV^\top + U\dot{S}V^\top + US\dot{V}^\top = \dot{A}VV^\top. \quad (13)$$

As is shown in the proof of Lemma 5.4 of [5] (see also [2]), the decomposition becomes unique if we impose that S stays block-diagonal,

$$S = \begin{pmatrix} S' & 0 \\ 0 & S'' \end{pmatrix},$$

and

$$U^\top \dot{U} = H, \quad V^\top \dot{V} = K$$

with $r \times r$ matrices of the block form

$$H = \begin{pmatrix} 0 & H_{12} \\ H_{21} & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & K_{12} \\ K_{21} & 0 \end{pmatrix},$$

which are skew-symmetric, $H_{12} = -H_{21}^\top$ and $K_{12} = -K_{21}^\top$. With the corresponding decompositions $U = (U', U'')$ and $V = (V', V'')$ the proof of Lemma 5.4 of [5] yields that

$$H_{12} = -(S')^{-\top} V'^\top \dot{A}^\top U'' + O(\varepsilon), \quad K_{12} = -(S')^{-1} U'^\top \dot{A} V'' + O(\varepsilon),$$

and in particular $H_{12} = O(1)$, $K_{12} = O(1)$. Multiplying (13) with U^\top from the left and with V from the right, we obtain

$$HS + \dot{S} + SK^\top = U^\top \dot{A} V,$$

which yields on the diagonal blocks

$$\dot{S}' = U'^\top \dot{A} V', \quad \dot{S}'' = U''^\top \dot{A} V''.$$

From (13) we further obtain

$$(U' S')^\bullet + U'' S'' K_{12}^\top = \dot{A} V'$$

and, using also the above equation for \dot{S}' ,

$$S' \dot{V}'^\top + H_{12} S'' V''^\top = U'^\top \dot{A} V'' V''^\top.$$

We show in part (b) of the proof below that $U''^\top \dot{A} V'' = O(\varepsilon + h)$ (but we cannot conclude the same for $U'^\top \dot{A} V''$). In summary, we get (indicating now the subscript I)

$$\begin{aligned} \dot{S}'_I &= U_I'^\top \dot{A} V_I', & \dot{S}''_I &= O(\varepsilon + h) \\ (U_I' S_I')^\bullet &= \dot{A} V_I' + O(\varepsilon + h) \\ S_I' \dot{V}_I'^\top &= U_I'^\top \dot{A} V_I'' V_I''^\top + O(\varepsilon + h). \end{aligned}$$

For the second step in the splitting we obtain similarly

$$\begin{aligned} \dot{S}''_I &= -U_I''^\top \dot{A} V_I', & \dot{S}''_I &= O(\varepsilon + h) \\ \dot{U}_I' S_I' &= -U_I'' U_I''^\top \dot{A} V_I' + O(\varepsilon + h) \\ S_I' \dot{V}_I'^\top &= -U_I''^\top \dot{A} V_I'' V_I''^\top + O(\varepsilon + h), \end{aligned}$$

and for the third step we obtain

$$\begin{aligned}\dot{S}'_{III} &= U'^{\top}_{III} \dot{A} V'_{III}, & \dot{S}''_{III} &= O(\varepsilon + h) \\ \dot{U}'_{III} S'_{III} &= U''_{III} U'^{\top}_{III} \dot{A} V'_{III} + O(\varepsilon + h) \\ (S'_{III} V'^{\top}_{III})^{\cdot} &= U'^{\top}_{III} \dot{A} + O(\varepsilon + h).\end{aligned}$$

Comparing these equations with those for $\bar{S}, \bar{U}, \bar{V}$ in the rank- q splitting method, it follows that

$$\begin{aligned}S'_1 &= S'_{III}(t_1) = \bar{S}_1 + O(h\varepsilon + h^2) \\ U'_1 &= U'_{III}(t_1) = \bar{U}_1 + O(h\varepsilon + h^2) \\ V'_1 &= V'_{III}(t_1) = \bar{V}_1 + O(h\varepsilon + h^2).\end{aligned}$$

Since stable error propagation in the rank- q splitting method is obtained by the standard argument using the Lipschitz continuity of the right-hand side of the differential equation (uniformly in ε), we conclude to the assertion of the theorem.

(b) We decompose the rank- q matrix

$$A'(t) = \hat{U}'(t) \hat{S}'(t) \hat{V}'(t)^{\top} \quad \text{with} \quad \hat{U}'(t) \dot{\hat{U}}'(t) = 0, \quad \hat{V}'(t) \dot{\hat{V}}'(t) = 0$$

and $\hat{U}'(t_0) = U'_0 + O(\varepsilon + h)$, $\hat{V}'(t_0) = V'_0 + O(\varepsilon + h)$. This choice of initial factors is possible because of the condition $A'(t_0) = Y_0 + O(\varepsilon + h)$, and the factorization at later t exists by solving the rank- q differential equations (5). For $t_0 \leq t \leq t_0 + h$ we have $U'(t) = U'(t_0) + O(h) = \hat{U}'(t_0) + O(\varepsilon + h) = \hat{U}'(t) + O(\varepsilon + h)$ and $V'(t) = \hat{V}'(t) + O(\varepsilon + h)$, and hence

$$\dot{A}'(t) = \dot{\hat{U}}'(t) \hat{S}'(t) V'(t)^{\top} + U'(t) \dot{\hat{S}}'(t) V'(t)^{\top} + U'(t) \hat{S}'(t) \dot{\hat{V}}'(t)^{\top} + O(\varepsilon + h).$$

Since $U''(t)^{\top} U'(t) = 0$ and $V''(t)^{\top} V'(t) = 0$, this yields the desired bound

$$U''(t)^{\top} \dot{A}(t) V''(t) = O(\varepsilon + h),$$

and the proof is complete. \square

5 Numerical experiments

5.1 Problem setting

The example is taken from [5]. We generate time-dependent matrices $A(t)$ as

$$A(t) = Q_1(t)(A_1 + \exp(t)A_2)Q_2(t),$$

where the orthogonal matrices $Q_1(t)$ and $Q_2(t)$ are generated as the solutions of differential equations

$$\dot{Q}_i = T_i Q_i, \quad i = 1, 2$$

with random skew-symmetric matrices T_i . The matrices A_1, A_2 are generated as follows. First, we generate a 10×10 matrix as an identity matrix plus a matrix with random entries distributed uniformly over $[0, 0.5]$. This matrix is then set as a leading block of a 100×100 matrix. After that, we add a perturbation to this enlarged matrix. The perturbation is generated as a matrix with uniformly distributed entries on $[0, \varepsilon]$. For small ε this matrix is close to a rank-10 matrix. If the rank of the approximation is chosen larger than 10, the norm of S^{-1} in (5) will be large and this leads to instability with standard time discretizations.

5.2 Numerical comparisons

We will compare the following schemes. The first scheme is the standard implicit midpoint rule combined with fixed point iteration applied directly to the system (5). We test the proposed splitting schemes with different orders of splitting and with/without symmetrization. We denote by KSL the scheme of Section 3.2, where first $K = US$ is updated, then S , then $L = VS^\top$. By KLS we denote the scheme where first K , then L , then S are updated. We thus consider the following methods:

1. KLS scheme (first order)
2. KLS scheme with symmetrization (second order)
3. KSL scheme (first order)
4. KSL scheme with symmetrization (second order)

We are interested in the approximation errors $\|Y(t) - A(t)\|$ for each particular scheme and different values of r and ε . The results are presented in Figure 1, where we also plot the error of the best rank- r approximation to $A(t)$ computed by SVD. Note that both KSL schemes perform remarkably better in the overapproximation case (subplot d). The midpoint rule is unstable in case d), whereas both KLS schemes have significantly higher error than the KSL schemes. All computations are done with constant step size $h = 10^{-3}$.

To test the convergence properties of the schemes with respect to the timestep h , we have computed the numerical order of the different schemes using the Runge rule:

$$\|y(h) - y(h/2)\| / \|y(h/2) - y(h/4)\| \approx 2^p \quad \text{in case of order } p.$$

	p	Appr. err.
Midpoint	2.0023	0.2200
KLS	1.0307	1.8133
KLS(symm)	1.8226	0.2215
KSL	1.0089	0.2188
KSL(symm)	2.005	0.2195

Table 1: $\varepsilon = 10^{-3}, r = 10$

	p	Appr. err.
Midpoint	2.0024	0.0188
KLS	1.0309	1.8030
KLS(symm)	1.8231	0.0324
KSL	1.0082	0.0002
KSL(symm)	2.0049	0.0002

Table 2: $\varepsilon = 10^{-6}, r = 10$

	p	Appr. err.
Midpoint	0.0001	0.1006
KLS	0.8154	1.4224
KLS(symm)	1.4911	0.3142
KSL	1.0354	0.0913
KSL(symm)	1.9929	0.0913

Table 3: $\varepsilon = 10^{-3}, r = 20$

	p	Appr. err.
Midpoint	-	failed
KLS	0.9633	1.3435
KLS(symm)	0.3127	1.5479
KSL	1.0362	9.1316e-05
KSL(symm)	1.993	9.1283e-05

Table 4: $\varepsilon = 10^{-6}, r = 20$

The approximation error listed is the error at $t = 1$ with respect to the given matrix $A(t)$, not with respect to the solution $Y(t)$ of rank r of the differential equations (5). In the overapproximation

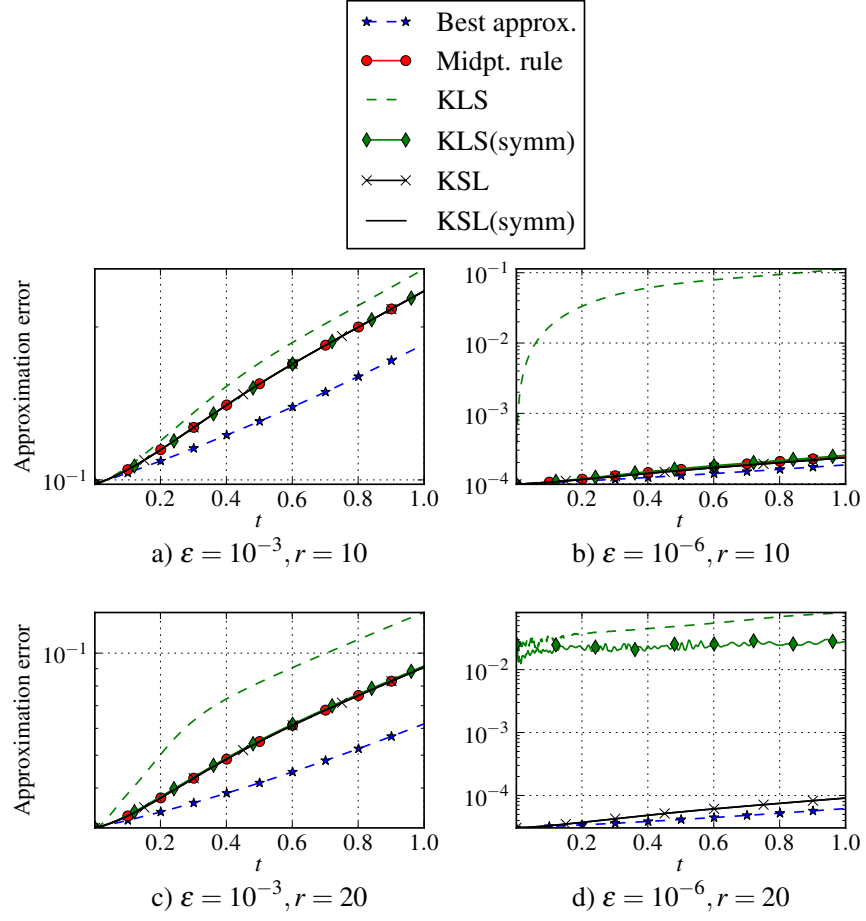


Figure 1: Dynamical low-rank approximation error for different schemes and different values of approximation rank r and perturbation size ε .

case both KLS schemes perform much worse, and the symmetrized version loses its second order. The KSL scheme, that is, the scheme of Section 3.2, and its symmetrized version (see Section 3.3) clearly outperform the other methods.

The last test describes the stability of the schemes with respect to the time step h . In Figure 2 we plot the approximation error at time $t = 1$ for both KSL schemes and the midpoint rule for different h ranging from 10^{-1} to 10^{-3} . The rank r was set to 20 (overapproximation case) and the noise level was chosen to be $\varepsilon = 10^{-3}$. The midpoint rule becomes unstable for large values of h ,

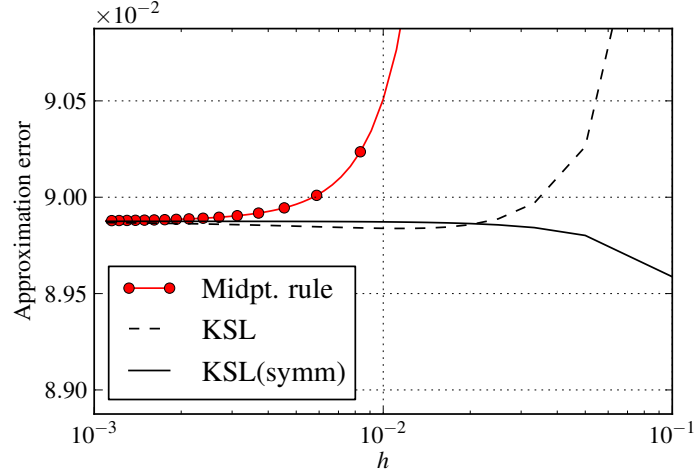


Figure 2: Dynamical low-rank approximation error for different schemes versus stepsize h , for $r = 20$ and $\varepsilon = 10^{-3}$

whereas both KSL schemes give a good result for the whole range of stepsizes. It is interesting to compare this value with the best low-rank approximation of $A(1)$. The error of the best rank-10 approximation of $A(1)$ (computed by the SVD) is approximately 10^{-2} and the error of the best rank-20 approximation is approximately $3 \cdot 10^{-3}$. The dynamical low-rank approximation thus captures the “smooth” component of the solution.

6 Conclusion and perspectives

We have proposed and analyzed a fully explicit, computationally inexpensive integrator for the dynamical low-rank approximation of time-dependent matrices that is based on splitting the projector onto the tangent space of the low-rank manifold. The integrator has remarkable robustness under over-approximation with a too high rank. While standard explicit and implicit integrators break down in such a situation, the integrator proposed here does not suffer from the ill-conditioning or singularity of the small matrix factor in the orthogonal low-rank factorization.

The robustness under overapproximation enables one to control the rank adaptively. Lowering the rank is trivial, but thanks to the robustness under a reduced rank we are able to raise the rank in a natural way, continuing the computations with the higher rank starting from the values of lower rank. This is not possible with standard integrators applied to the higher-rank differential equations, which would have to start from a singular matrix factor, in which case the differential equations are not well-defined.

Another application of the proposed integrator is in optimization algorithms on a low-rank manifold, such as cg or Newton’s method. There, an update $A + \Delta A$ to a low-rank iterate A has to

be truncated (or retracted in another terminology) back to the given low rank. This can be done efficiently by applying one step of our integrator to $A + t\Delta A$ at $t = 1$.

The integrator can be extended to the low-rank approximation of tensors in the tensor train and hierarchical Tucker formats. This extension will be studied in forthcoming work.

References

- [1] A. Arnold and T. Jahnke, On the approximation of high-dimensional differential equations in the hierarchical Tucker format, tech. rep., KIT, Karlsruhe, 2012.
- [2] L. Dieci and T. Eirola, On smooth decompositions of matrices, *SIAM J. Numer. Anal.* **20**, 800–819 (1999).
- [3] W. Hackbusch and S. Kühn, A new scheme for the tensor representation, *J. Fourier Anal. Appl.* **15**, 706–722 (2009).
- [4] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration*, Springer-Verlag, Berlin, second ed., 2006.
- [5] O. Koch and C. Lubich, Dynamical low-rank approximation, *SIAM J. Matrix Anal. Appl.* **29**, 434–454 (2007).
- [6] ———, Dynamical tensor approximation, *SIAM J. Matrix Anal. Appl.* **31**, 2360–2375 (2010).
- [7] C. Lubich, *From quantum to classical molecular dynamics: reduced models and numerical analysis*, European Math. Soc., Zurich, 2008.
- [8] C. Lubich, T. Rohwedder, R. Schneider, and B. Vandereycken, Dynamical approximation of hierarchical Tucker and tensor-train tensors, Preprint 126, DFG SPP 1324, 2012.
- [9] R. I. McLachlan and G. R. W. Quispel, Splitting methods, *Acta Numer.* **11**, 341–434 (2002).
- [10] H. Meyer, F. Gatti, and G. Worth (eds.), *Multidimensional Quantum Dynamics: MCTDH Theory and Applications*, Wiley, New York, 2009.
- [11] H. Meyer, U. Manthe, and L. S. Cederbaum, The multi-configurational time-dependent Hartree approach, *Chemical Physics Letters* **165**, 73–78(1990).
- [12] A. Nonnenmacher and C. Lubich, Dynamical low-rank approximation: applications and numerical experiments, *Math. Comput. Simulation* **79**, 1346–1357 (2008).
- [13] I. V. Oseledets, Tensor-train decomposition, *SIAM J. Sci. Comput.* **33**, 2295–2317 (2011).
- [14] I. V. Oseledets, B. N. Khoromskij, and R. Schneider, Efficient time-stepping scheme for dynamics on TT-manifolds, Preprint 24, MPI MIS, 2012.